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Bis(pyridine-2-carboxylato-κ^2N,O)copper(II)]–benzene-1,3,5-tricarboxylic acid–water (1/2/2)

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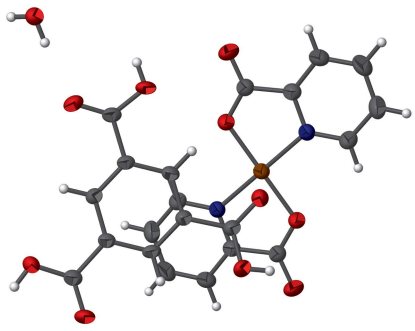
Keywords: crystal structure; mixed ligands coordination polymer; copper carboxylates; hydrogen bond.

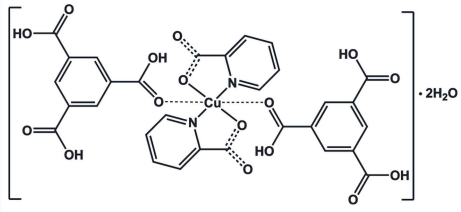
Structural data: full structural data are available from iucrdata.iucr.org

In the title complex, $[Cu(C_6H_4O_2N)_2]\cdot 2C_9H_6O_6\cdot 2H_2O$, the Cu^{2+} ion lies on a center of inversion and coordinates with symmetry related pyridine nitrogen and carboxyl oxygen atoms from two pyridine-2-carboxylic acid anions, giving rise to a square-planar coordination geometry. There are weak axial bonds between Cu and an O atom of a symmetry-related trimesic acid moieties [Cu···O = 2.837 (2) Å] The Cu···O weak interactions and hydrogen bonds stabilize the whole structure.

3D view



Chemical scheme



Structure description

The asymmetric unit of the title compound contains half copper center, one pyridine-2-carboxylic acid anion, one BTC (benzene-1,3,5-tricarboxylic acid) ligand and one crystal water molecule (Fig. 1). The Cu^{2+} ion lies on the symmetry center and is coordinated by two symmetry-related pyridine nitrogen atoms and two symmetry-related carboxyl oxygen atoms, giving rise to a square-planar coordination geometry. In the axial position, a very weak interaction Cu1···O3 [2.837 (2) Å] is observed. Interestingly, the 1,4-bis(3-pyridyl)-2,3-diaza-1,3-butadiene ligand decomposed during the hydrothermal process and is oxidized into pyridine-2-carboxylic acid. According to our earlier research, the occurrence of oxidation may be caused by excess of Cu^{II} salt, which may act as an oxidative agent to promote the formation of the carboxyl group (Sun *et al.*, 2016). Each pyridine-2-carboxylic acid anion coordinates with one Cu^{2+} ion in a bidentate *N*,*O*-chelated mode, forming a five-membered ring.

In the crystal, C—H···O and O—H···O hydrogen bonds (Table 1) and together with weak Cu···O interactions link the complex molecules into a three-dimensional frame-

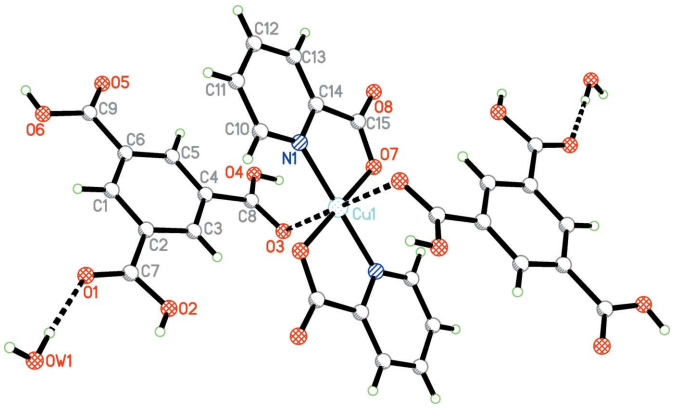


Figure 1
The title compound showing the atom-labelling scheme with displacement ellipsoids drawn at the 30% probability level. Unlabelled atoms are generated by the symmetry operation $-x$, $-y$, $-z$. Hydrogen bonds are shown by dashed lines

work (Fig. 2). Although the O1···C9 and O6···C7 distances [3.002 (3)and 3.014 (3) Å, respectively] between the two symmetry-related BTC^{3-} ligands (symmetry code: $-x$, $-y$, $-1-z$) are short, there are no π–π interactions because the inter-centroid distance between the two benzene rings is 5.4029 (15) Å, which is much larger than the normal π–π stacking distance of 3.3–3.8 Å. The shortest distance between the two carbon atoms (C1 and C1′) is 3.379 (4) Å. The other C···C distances of the two rings are longer than 3.94 Å. In addition, the distance between the centroid of one benzene ring and the C atoms of another is longer than 4.28 Å.

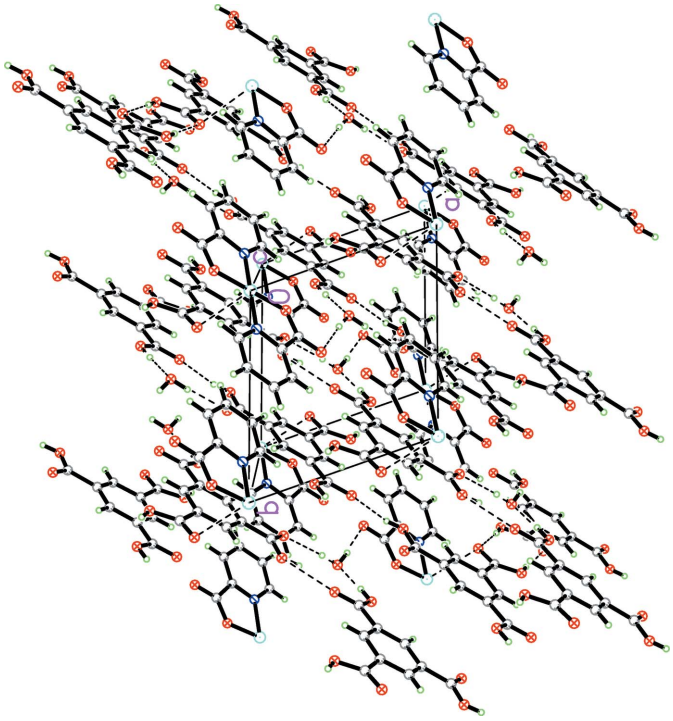


Figure 2
The packing of the title compound. Hydrogen bonds and Cu···O interactions are shown as dashed lines.

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
O2—H2···O5^{i}	0.82	1.84	2.621 (2)	158
O4—H4···O3^{ii}	0.82	1.85	2.659 (3)	167
O6—H6···O*W*1^{iii}	0.82	1.73	2.553 (3)	176
C10—H10···O7^{iv}	0.93	2.66	3.121 (3)	112
C13—H13···O4^{v}	0.93	2.61	3.454 (4)	152
O*W*1—H*W*1*A*···O8^{vi}	0.85	1.88	2.729 (3)	174
O*W*1—H*W*1*A*···O7^{vi}	0.85	2.66	3.259 (3)	129
O*W*1—H*W*1*B*···O1	0.85	2.02	2.872 (3)	175

Symmetry codes: (i) $x-1, y-1, z$; (ii) $-x+1, -y, -z$; (iii) $x+1, y+1, z$; (iv) $-x, -y, -z$; (v) $-x+1, -y+1, -z$; (vi) $x-1, y-1, z-1$.

Table 2
Experimental details.

Crystal data	
Chemical formula	$[Cu(C_6H_4NO_2)_2]\cdot 2C_9H_6O_6\cdot 2H_2O$
M_r	764.05
Crystal system, space group	Triclinic, $P\overline{1}$
Temperature (K)	296
a, b, c (Å)	7.9262 (6), 8.5356 (6), 12.3629 (9)
α, β, γ (°)	107.081 (2), 90.644 (2), 108.679 (2)
V (Å^3)	752.26 (10)
Z	1
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.82
Crystal size (mm)	0.31 × 0.14 × 0.12
Data collection	
Diffractometer	Bruker APEXII CCD
Absorption correction	Multi-scan (*SADABS*; Bruker, 2015)
T_{min}, T_{max}	0.639, 0.746
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	14996, 3473, 2501
R_{int}	0.062
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.651
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.047, 0.123, 1.06
No. of reflections	3473
No. of parameters	238
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.41, −0.46

Computer programs: *APEX2* and *SAINT* (Bruker, 2015), *SHELXTL* (Sheldrick, 2008) and *SHELXL2014/7* (Sheldrick, 2015).

Synthesis and crystallization

A mixture of trimesic acid (21 mg, 0.1 mmol), 1,4-bis(3-pyridyl)-2,3-diaza-1,3-butadiene (2-bpdb, 11 mg, 0.05 mmol) and $CuCl_2\cdot 2H_2O$ (51 mg, 0.3 mmol) in 5 mL of distilled H_2O was stirred for 10 min in air, and then the mixture was turned into a Parr Teflon-lined stainless steel vessel and heated at 160°C for 60 h. Dark-red crystals suitable for X-ray diffraction were obtained in a yield of 78% (based on $CuCl_2\cdot 2H_2O$).

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2.

Funding information

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full crystallographic data

IUCrData (2021). **6**, x210672 [https://doi.org/10.1107/S2414314621006726]

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Wenkai Zhang, Bingguang Zhang and Qiaozhen Sun

Bis(pyridine-2-carboxylato-κ^2N,O)copper(II)]–benzene-1,3,5-tricarboxylic acid–water (1/2/2)

Crystal data

$[Cu(C_6H_4NO_2)_2]\cdot 2C_9H_6O_6\cdot 2H_2O$
M_r = 764.05
Triclinic, $P\overline{1}$
a = 7.9262 (6) Å
b = 8.5356 (6) Å
c = 12.3629 (9) Å
α = 107.081 (2)°
β = 90.644 (2)°
γ = 108.679 (2)°
V = 752.26 (10) Å^3
Z = 1
$F(000)$ = 391
D_x = 1.687 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 5514 reflections
θ = 3.1–26.9°
μ = 0.82 mm^{-1}
T = 296 K
Prism, red
0.31 × 0.14 × 0.12 mm

Data collection

Bruker APEXII CCD diffractometer
phi and ω scans
Absorption correction: multi-scan (SADABS; Bruker, 2015)
T_{min} = 0.639, T_{max} = 0.746
14996 measured reflections
3473 independent reflections
2501 reflections with $I > 2\sigma(I)$
R_{int} = 0.062
θ_{max} = 27.6°, θ_{min} = 3.1°
h = −10→10
k = −11→11
l = −16→16

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.047
$wR(F^2)$ = 0.123
S = 1.06
3473 reflections
238 parameters
0 restraints
Hydrogen site location: mixed
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0543P)^2 + 0.4521P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.41 e Å^{-3}
$\Delta\rho_{min}$ = −0.46 e Å^{-3}

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Refinement. All of the non-hydrogen atoms were refined with anisotropic thermal displacement coefficients. Hydrogen atoms attached to the carbons were placed in their calculated position and refined with a idealized riding model. Those attached to oxygen were first located in a difference Fourier and then refined with a idealized riding model [U_{iso}(H) = 1.2U_{eq}(C) or 1.5 U_{eq}(O)].

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
Cu1	0.0000	0.0000	0.0000	0.04024 (18)
O1	−0.1595 (2)	−0.3787 (3)	−0.56042 (16)	0.0418 (5)
O2	−0.1580 (3)	−0.4334 (3)	−0.39491 (18)	0.0456 (5)
H2	−0.2531	−0.5104	−0.4252	0.068*
O3	0.2978 (3)	−0.0951 (3)	−0.08146 (16)	0.0428 (5)
O4	0.5456 (3)	0.0969 (3)	−0.10936 (18)	0.0500 (6)
H4	0.5797	0.0972	−0.0464	0.075*
O5	0.5473 (3)	0.2951 (3)	−0.44481 (17)	0.0453 (5)
O6	0.3404 (2)	0.1325 (2)	−0.59294 (15)	0.0367 (4)
H6	0.4000	0.2025	−0.6230	0.055*
O7	0.1869 (3)	0.1722 (2)	0.11419 (16)	0.0457 (5)
O8	0.3797 (3)	0.4424 (3)	0.15484 (19)	0.0594 (6)
N1	0.0395 (3)	0.1833 (3)	−0.07130 (18)	0.0344 (5)
C1	0.1570 (3)	−0.0820 (3)	−0.4716 (2)	0.0275 (5)
H1	0.1094	−0.1022	−0.5455	0.033*
C2	0.0714 (3)	−0.1918 (3)	−0.4104 (2)	0.0263 (5)
C3	0.1436 (3)	−0.1621 (3)	−0.3011 (2)	0.0294 (6)
H3	0.0860	−0.2343	−0.2595	0.035*
C4	0.3020 (3)	−0.0248 (3)	−0.2530 (2)	0.0281 (5)
C5	0.3855 (3)	0.0857 (3)	−0.3140 (2)	0.0291 (6)
H5	0.4904	0.1787	−0.2815	0.035*
C6	0.3125 (3)	0.0574 (3)	−0.4232 (2)	0.0268 (5)
C7	−0.0944 (3)	−0.3437 (3)	−0.4643 (2)	0.0296 (6)
C8	0.3841 (3)	−0.0081 (3)	−0.1403 (2)	0.0318 (6)
C9	0.4110 (3)	0.1745 (3)	−0.4883 (2)	0.0299 (6)
C10	−0.0462 (4)	0.1813 (4)	−0.1655 (2)	0.0417 (7)
H10	−0.1388	0.0809	−0.2067	0.050*
C11	−0.0005 (5)	0.3247 (4)	−0.2033 (3)	0.0509 (8)
H11	−0.0636	0.3222	−0.2680	0.061*
C12	0.1394 (5)	0.4710 (4)	−0.1440 (3)	0.0555 (9)
H12	0.1745	0.5675	−0.1696	0.067*
C13	0.2268 (4)	0.4741 (4)	−0.0469 (3)	0.0479 (8)
H13	0.3214	0.5726	−0.0056	0.058*
C14	0.1726 (4)	0.3293 (4)	−0.0113 (2)	0.0363 (6)
C15	0.2557 (4)	0.3172 (4)	0.0947 (2)	0.0396 (7)
OW1	−0.4676 (3)	−0.6609 (3)	−0.69195 (17)	0.0420 (5)
HW1A	−0.5227	−0.6321	−0.7381	0.063*
HW1B	−0.3783	−0.5734	−0.6547	0.063*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cu1	0.0481 (3)	0.0303 (3)	0.0334 (3)	−0.0012 (2)	−0.0049 (2)	0.0132 (2)
O1	0.0319 (10)	0.0412 (11)	0.0375 (11)	−0.0042 (9)	−0.0068 (8)	0.0094 (9)
O2	0.0320 (11)	0.0391 (11)	0.0521 (12)	−0.0131 (9)	−0.0084 (9)	0.0227 (10)
O3	0.0393 (11)	0.0464 (12)	0.0345 (11)	−0.0023 (9)	−0.0033 (8)	0.0197 (9)
O4	0.0395 (11)	0.0524 (13)	0.0460 (12)	−0.0101 (10)	−0.0180 (9)	0.0269 (10)
O5	0.0347 (11)	0.0398 (11)	0.0472 (12)	−0.0118 (9)	−0.0043 (9)	0.0202 (9)
O6	0.0364 (11)	0.0366 (11)	0.0319 (10)	0.0004 (8)	0.0015 (8)	0.0167 (8)
O7	0.0544 (13)	0.0332 (11)	0.0388 (11)	−0.0032 (9)	−0.0106 (9)	0.0162 (9)
O8	0.0581 (14)	0.0435 (13)	0.0561 (14)	−0.0120 (11)	−0.0223 (11)	0.0188 (11)
N1	0.0386 (13)	0.0311 (12)	0.0292 (12)	0.0051 (10)	0.0015 (9)	0.0104 (9)
C1	0.0235 (12)	0.0282 (13)	0.0282 (13)	0.0060 (10)	−0.0004 (10)	0.0084 (10)
C2	0.0204 (12)	0.0231 (12)	0.0328 (13)	0.0043 (10)	0.0006 (10)	0.0085 (10)
C3	0.0253 (13)	0.0264 (13)	0.0352 (14)	0.0033 (10)	0.0021 (10)	0.0140 (11)
C4	0.0266 (13)	0.0259 (12)	0.0291 (13)	0.0048 (10)	−0.0011 (10)	0.0095 (10)
C5	0.0210 (12)	0.0235 (12)	0.0368 (14)	0.0002 (10)	−0.0031 (10)	0.0092 (10)
C6	0.0222 (12)	0.0245 (12)	0.0333 (13)	0.0051 (10)	0.0014 (10)	0.0116 (10)
C7	0.0213 (12)	0.0263 (13)	0.0388 (15)	0.0045 (10)	0.0009 (11)	0.0107 (11)
C8	0.0286 (14)	0.0294 (13)	0.0322 (14)	0.0021 (11)	−0.0030 (11)	0.0106 (11)
C9	0.0259 (13)	0.0275 (13)	0.0362 (14)	0.0068 (11)	0.0033 (11)	0.0124 (11)
C10	0.0466 (17)	0.0358 (16)	0.0341 (15)	0.0054 (13)	−0.0028 (12)	0.0083 (12)
C11	0.069 (2)	0.0491 (19)	0.0354 (16)	0.0176 (17)	−0.0004 (15)	0.0176 (14)
C12	0.076 (2)	0.0401 (17)	0.0501 (19)	0.0084 (17)	0.0044 (17)	0.0258 (15)
C13	0.0525 (18)	0.0347 (16)	0.0460 (18)	−0.0019 (14)	−0.0004 (14)	0.0158 (13)
C14	0.0352 (15)	0.0346 (15)	0.0347 (15)	0.0056 (12)	0.0037 (11)	0.0112 (12)
C15	0.0407 (16)	0.0376 (16)	0.0331 (15)	0.0033 (13)	−0.0006 (12)	0.0115 (12)
OW1	0.0400 (12)	0.0408 (11)	0.0403 (12)	0.0014 (9)	−0.0043 (9)	0.0192 (9)

Geometric parameters (Å, º)

Cu1—O7^{i}	1.9204 (18)	C2—C3	1.380 (3)
Cu1—O7	1.9204 (18)	C2—C7	1.495 (3)
Cu1—N1^{i}	1.956 (2)	C3—C4	1.391 (3)
Cu1—N1	1.956 (2)	C3—H3	0.9300
Cu1—O3	2.837 (2)	C4—C5	1.388 (3)
O1—C7	1.203 (3)	C4—C8	1.479 (3)
O2—C7	1.313 (3)	C5—C6	1.385 (3)
O2—H2	0.8200	C5—H5	0.9300
O3—C8	1.246 (3)	C6—C9	1.497 (3)
O4—C8	1.281 (3)	C10—C11	1.379 (4)
O4—H4	0.8200	C10—H10	0.9300
O5—C9	1.210 (3)	C11—C12	1.373 (4)
O6—C9	1.303 (3)	C11—H11	0.9300
O6—H6	0.8200	C12—C13	1.369 (4)
O7—C15	1.278 (3)	C12—H12	0.9300
O8—C15	1.227 (3)	C13—C14	1.374 (4)

N1—C10	1.335 (3)	C13—H13	0.9300
N1—C14	1.347 (3)	C14—C15	1.505 (4)
C1—C6	1.385 (3)	OW1—HW1A	0.8499
C1—C2	1.390 (3)	OW1—HW1B	0.8499
C1—H1	0.9300		

O7^{i}—Cu1—O7	180.0 (2)	C4—C5—H5	120.0
O7^{i}—Cu1—N1^{i}	84.32 (8)	C5—C6—C1	119.8 (2)
O7—Cu1—N1^{i}	95.68 (8)	C5—C6—C9	118.4 (2)
O7^{i}—Cu1—N1	95.68 (8)	C1—C6—C9	121.7 (2)
O7—Cu1—N1	84.32 (8)	O1—C7—O2	124.7 (2)
N1^{i}—Cu1—N1	180.0	O1—C7—C2	123.2 (2)
O7^{i}—Cu1—O3	99.58 (8)	O2—C7—C2	112.1 (2)
O7—Cu1—O3	80.42 (8)	O3—C8—O4	123.3 (2)
N1^{i}—Cu1—O3	85.19 (8)	O3—C8—C4	120.2 (2)
N1—Cu1—O3	94.81 (8)	O4—C8—C4	116.4 (2)
C7—O2—H2	109.5	O5—C9—O6	124.5 (2)
C8—O3—Cu1	113.90 (18)	O5—C9—C6	120.8 (2)
C8—O4—H4	109.5	O6—C9—C6	114.7 (2)
C9—O6—H6	109.5	N1—C10—C11	121.5 (3)
C15—O7—Cu1	114.81 (17)	N1—C10—H10	119.2
C10—N1—C14	119.2 (2)	C11—C10—H10	119.2
C10—N1—Cu1	129.42 (19)	C12—C11—C10	119.1 (3)
C14—N1—Cu1	111.42 (18)	C12—C11—H11	120.5
C6—C1—C2	120.5 (2)	C10—C11—H11	120.5
C6—C1—H1	119.8	C13—C12—C11	119.6 (3)
C2—C1—H1	119.8	C13—C12—H12	120.2
C3—C2—C1	119.5 (2)	C11—C12—H12	120.2
C3—C2—C7	120.5 (2)	C12—C13—C14	119.0 (3)
C1—C2—C7	120.0 (2)	C12—C13—H13	120.5
C2—C3—C4	120.4 (2)	C14—C13—H13	120.5
C2—C3—H3	119.8	N1—C14—C13	121.6 (3)
C4—C3—H3	119.8	N1—C14—C15	114.3 (2)
C5—C4—C3	119.9 (2)	C13—C14—C15	124.1 (3)
C5—C4—C8	121.4 (2)	O8—C15—O7	125.4 (3)
C3—C4—C8	118.6 (2)	O8—C15—C14	119.5 (3)
C6—C5—C4	120.0 (2)	O7—C15—C14	115.1 (2)
C6—C5—H5	120.0	HW1A—OW1—HW1B	109.5

C6—C1—C2—C3	−0.7 (4)	C5—C6—C9—O5	−2.9 (4)
C6—C1—C2—C7	−178.8 (2)	C1—C6—C9—O5	−179.6 (2)
C1—C2—C3—C4	−0.8 (4)	C5—C6—C9—O6	175.6 (2)
C7—C2—C3—C4	177.3 (2)	C1—C6—C9—O6	−1.1 (4)
C2—C3—C4—C5	1.7 (4)	C14—N1—C10—C11	0.6 (4)
C2—C3—C4—C8	−174.1 (2)	Cu1—N1—C10—C11	179.5 (2)
C3—C4—C5—C6	−1.0 (4)	N1—C10—C11—C12	1.7 (5)
C8—C4—C5—C6	174.6 (2)	C10—C11—C12—C13	−2.1 (5)
C4—C5—C6—C1	−0.5 (4)	C11—C12—C13—C14	0.3 (5)

C4—C5—C6—C9	−177.2 (2)	C10—N1—C14—C13	−2.4 (4)
C2—C1—C6—C5	1.3 (4)	Cu1—N1—C14—C13	178.4 (2)
C2—C1—C6—C9	178.0 (2)	C10—N1—C14—C15	178.5 (2)
C3—C2—C7—O1	−177.5 (3)	Cu1—N1—C14—C15	−0.6 (3)
C1—C2—C7—O1	0.6 (4)	C12—C13—C14—N1	2.0 (5)
C3—C2—C7—O2	2.0 (3)	C12—C13—C14—C15	−179.1 (3)
C1—C2—C7—O2	−179.9 (2)	Cu1—O7—C15—O8	−177.8 (3)
Cu1—O3—C8—O4	113.7 (3)	Cu1—O7—C15—C14	2.5 (3)
Cu1—O3—C8—C4	−67.3 (3)	N1—C14—C15—O8	179.1 (3)
C5—C4—C8—O3	171.8 (3)	C13—C14—C15—O8	0.1 (5)
C3—C4—C8—O3	−12.5 (4)	N1—C14—C15—O7	−1.2 (4)
C5—C4—C8—O4	−9.2 (4)	C13—C14—C15—O7	179.7 (3)
C3—C4—C8—O4	166.5 (2)		

Symmetry code: (i) −*x*, −*y*, −*z*.

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O2—H2···O5^{ii}	0.82	1.84	2.621 (2)	158
O4—H4···O3^{iii}	0.82	1.85	2.659 (3)	167
O6—H6···O*W*1^{iv}	0.82	1.73	2.553 (3)	176
C10—H10···O7^{i}	0.93	2.66	3.121 (3)	112
C13—H13···O4^{v}	0.93	2.61	3.454 (4)	152
O*W*1—H*W*1*A*···O8^{vi}	0.85	1.88	2.729 (3)	174
O*W*1—H*W*1*A*···O7^{vi}	0.85	2.66	3.259 (3)	129
O*W*1—H*W*1*B*···O1	0.85	2.02	2.872 (3)	175

Symmetry codes: (i) −*x*, −*y*, −*z*; (ii) *x*−1, *y*−1, *z*; (iii) −*x*+1, −*y*, −*z*; (iv) *x*+1, *y*+1, *z*; (v) −*x*+1, −*y*+1, −*z*; (vi) *x*−1, *y*−1, *z*−1.